Propane, 1,1,3,3-tetramethoxy-102-52-3 | DTXSID4059255

Model Performance

| Mode | Data |
|------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (| Training (75%) | | Test (25%) | |
|-----------------|------|------------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 | |

Model Results

Predicted value: -34.2 °C

Global applicability domain: Inside

Local applicability domain index: 5.69e-01

Confidence level: 6.72e-01

Nearest Neighbors from the Training Set

Image not found

Triethylene glycol dimethyl ether

Measured: -45.0 Predicted: -39.7

Image not found

Tetramethyl orthocarbonate

Measured: -5.00 **Predicted:** -17.8

Image not found

Bis(2-methoxyethyl) ether

Measured: -68.0 Predicted: -51.9

Image not found

2-(2-Ethoxyethoxy)ethyl acetate

Measured: -25.0 Predicted: -25.7

Image not found

2-(2-Butoxyethoxy)ethyl acetate

Measured: -32.0 Predicted: -24.5